

Modeling and Simulation for Nuclear Energy Workshop
 Los Alamos National Laboratory, Study Center (Jemez and Cochiti Rooms)
 July 29-30, 2008

Tuesday, July 29

8:00 Welcome and workshop objectives, Stephen Lee (CCS-DO)

8:15 Opportunities, Duncan McBranch (PADSTE)

8:30 – 12:00 Session A: Programmatic Internal and External Opportunities

Chair: Sara Scott (SPO-CNP)

Program managers will discuss current programs, players at local and national level, the organization of various programs, and upcoming opportunities in these programs. This session will include a discussion of opportunities in the industrial space as well as an examination of competitors and collaborators.

8:30 Overview of Civilian Nuclear Programs, Sara Scott (SPO-CNP)

9:00 Advanced Fuels Program Opportunities, Cetin Unal (X-4)

9:30 Industrial Opportunities, Ning Li (MPA-10)

10:00 MaRIE, Paul Follansbee (MST-DO)

10:15 Discussions and Q&A

12:00 Break for lunch

1:00 – 5:00 Session B: Integrated Codes

Chair: Mark Schraad (T-3)

This session will provide information on integrated codes we have at Los Alamos that can contribute to modeling and simulation for nuclear energy. The status of the codes, how they have (or can) be applied, and issues moving forward will be discussed.

1:00 Telluride, Bryan Lally (CCS-2)

1:15 MCNP and MCNP/X, Forrest Brown (X-3)

1:30 Crestone Project Code Suite, Mike Steinkamp (X-3)

1:45 PARTISN/Capsaicin, Randy Baker (CCS-2)

2:00 Cinder, Shannon T. Holloway (T-16)

2:15 PFLOTRAN, Peter Lichtner (EES-6)

2:30 Shavano, Scott Runnels (X-3)

2:45 TRACE/TRAC, D.V. Rao (D-DO)

3:00 CHAD, Mark Schraad (T-3)

3:15 McGNASH Code Development, Mark Chadwick (T-DO)

3:30 Economic Modeling, Sam Flaim (D-6)

3:45 Discussions and Q&A

5:00 Adjourn

Wednesday, July 30**8:30 – 12:30 Session C: Advanced Theory, Models, and Numerical Methods**

Chair: John Wills (T-17)

This is a broad area that speaks to a plethora of “science” capabilities that have been or can be brought to bear on the nuclear energy enterprise. Included here are fuels and materials multiscale, transport theory and methods, nuclear data, fission theory, analysis of seismic impact on nuclear facilities, modeling and simulation for environmental impact, and so on.

- 8:30 Multi-scale materials modeling for nuclear fuels, John Wills (T-17)
- 8:45 First-principles calculations for nuclear fuels, Sven Rudin (T-17)
- 9:00 Atomistic modeling of oxide materials, Steve Valone (MST-8)
- 9:15 Atomistic modeling of large/complex systems, Tim Germann (T-12)
- 9:30 Accelerated dynamics and kinetic Monte Carlo, Blas Uberuaga (MST-8)
- 9:45 Modeling phase stability in nuclear fuels, Marius Stan (CCS-2)
- 10:00 Nuclear Physics, Anna Hayes-Sterbenz (T-16)
- 10:15 Nuclear Data, Bob Little (X-1)
- 10:30 Radiation transport, Todd Urbatsch (CCS-2)
- 10:45 Validation opportunities using MaRIE: a preliminary discussion, Mark Bourke (MST-8)
- 11:00 Quantum chemistry approaches for nuclear energy systems, Enrique Batista (T-12)
- 11:15 Monte Carlo approaches to nuclear criticality, James Gubernatis (T-11)
- 11:30 Data and Visualization for Energy Futures, Jim Ahrens (CCS-1)
- 11:45 Lattice Boltzmann Method, Qinjun Kang (EES-6)
- 12:00 Discussions and Q&A

12:30 Break for lunch

2:00 – 5:00 Session D: Vision and Strategic Directions

Chair: Stephen Lee (CCS-DO)

This session will review, contrast and discuss existing visions related to models and simulations for nuclear energy. The speakers will emphasize LANL’s leadership role and the impact of the respective vision on LANL mission goals and strategic directions. The final discussion will provide a forum for commenting on the existing visions and proposing new, innovative LANL vision elements.

- 2:00 GNEP Roadmap and program perspective, NEAMS, Cetin Unal (X-4)
- 2:40 WPMM, International Perspective, Marius Stan (CCS-2)
- 3:00 Discussion: LANL vision on modeling and simulation for nuclear energy

During this discussion, session chairs, speakers, and other participants will discuss and agree on a set of action items related to:

- Writing the LANL Models and Simulation for Nuclear Energy report.
- Creating a set of overview presentations to be used for conferences, meetings with sponsors and other DOE representatives.
- Creating strong proposals in response to DOE, GENP, BES, LDRD and other upcoming calls.

5:00 Adjourn